yes - keep duplicate file here.

RESOURCE - RELATED RESEARCH

COMPUTERS AND CHEMISTRY

(RR-00612 COMPETING RENEWAL APPLICATION)

Submitted to

BIOTECHNOLOGY RESOURCES BRANCH

OF THE

NATIONAL INSTITUTES OF HEALTH

May, 1976

site visit 1/7/77

DEPARTMENTS OF

CHEMISTRY, GENETICS, AND COMPUTER SCIENCE

STANFORD UNIVERSITY

SECTION I

Form Approved
O.M.B. 68-R0249

DEPARTMENT OF
HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

GRANT APPLICATION

LEAVE BLANK

TYPE	PROGRAM	NUMBER
REVIEW GROUP		FORMERLY
COUNCIL *(Month, Year)*		DATE RECEIVED

TO BE COMPLETED BY PRINCIPAL INVESTIGATOR *(Items 1 through 7 and 15A)*

1. TITLE OF PROPOSAL *(Do not exceed 53 typewriter spaces)*
RESOURCE-RELATED RESEARCH - COMPUTERS AND CHEMISTRY

2. PRINCIPAL INVESTIGATOR

2A. NAME *(Last, First, Initial)*
Djerassi, Carl

2B. TITLE OF POSITION
Professor of Chemistry

2C. MAILING ADDRESS *(Street, City, State, Zip Code)*
Department of Chemistry
Stanford University
Stanford, California 94305

2D. DEGREE
Ph.D.

2E. SOCIAL SECURITY NO.
[redacted]

2F. TELEPHONE DATA
Area Code 415 TELEPHONE [redacted] EXTENSION

2G. DEPARTMENT, SERVICE, LABORATORY OR EQUIVALENT *(See Instructions)*
Department of Chemistry

2H. MAJOR SUBDIVISION *(See Instructions)*
Department of Humanities and Sciences

3. DATES OF ENTIRE PROPOSED PROJECT PERIOD *(This application)*

FROM	THROUGH
5/1977	4/1982

4. TOTAL DIRECT COSTS REQUESTED FOR PERIOD IN ITEM 3
$1,463,940

5. DIRECT COSTS REQUESTED FOR FIRST 12-MONTH PERIOD
$250,650

6. PERFORMANCE SITE(S) *(See Instructions)*
Department of Genetics,
Department of Chemistry, and
Department of Computer Science
Stanford University

7. Research Involving Human Subjects *(See Instructions)*
A. [X] NO B. [ ] YES Approved: _____ Date
C. [ ] YES – Pending Review

8. Inventions *(Renewal Applicants Only - See Instructions)*
A. [X] NO B. [ ] YES – Not previously reported
C. [ ] YES – Previously reported

TO BE COMPLETED BY RESPONSIBLE ADMINISTRATIVE AUTHORITY *(Items 8 through 13 and 15B)*

9. APPLICANT ORGANIZATION(S) *(See Instructions)*
Stanford University
Stanford, California 94305
IRS No. 94-1156365
Congressional District No. 12

10. NAME, TITLE, AND TELEPHONE NUMBER OF OFFICIAL(S) SIGNING FOR APPLICANT ORGANIZATION(S)
c/o Sponsored Projects Office
Telephone Number (s) (415) 497-2883

11. TYPE OF ORGANIZATION *(Check applicable item)*
[ ] FEDERAL [ ] STATE [ ] LOCAL [X] OTHER *(Specify)*
Private, non-profit University

12. NAME, TITLE, ADDRESS, AND TELEPHONE NUMBER OF OFFICIAL IN BUSINESS OFFICE WHO SHOULD ALSO BE NOTIFIED IF AN AWARD IS MADE
K. D. Creighton
Deputy Vice Pres. for Business & Finance
Stanford University
Stanford, California 94305
Telephone Number (415)497-2251

13. IDENTIFY ORGANIZATIONAL COMPONENT TO RECEIVE CREDIT FOR INSTITUTIONAL GRANT PURPOSES *(See Instructions)*
20 School of Humanities and Sciences

14. ENTITY NUMBER (Formerly PHS Account Number)
1941156365A1

15. CERTIFICATION AND ACCEPTANCE. We, the undersigned, certify that the statements herein are true and complete to the best of our knowledge and accept, as to any grant awarded, the obligation to comply with Public Health Service terms and conditions in effect at the time of the award.

SIGNATURES (Signatures required on original copy only. *Use ink. "Per" signatures not acceptable)*	A. SIGNATURE OF PERSON NAMED IN ITEM 2A	DATE See page 55A
	B. SIGNATURE(S) OF PERSON(S) NAMED IN ITEM 10	DATE

NIH 398 (FORMERLY PHS 398)

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE (Mo., Day, Yr.)
CARL DJERASSI	Professor of Chemistry	10/29/23
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Vienna, Austria	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Kenyon College	A.B. (summa cum laude)	1942	Chemistry, Biology
University of Wisconsin	Ph.D.	1945	Organic Chemistry Biochemistry (minor)

HONORS National Medal of Science ('73); Perkin Medal ('75); Am.Chem.Soc. Awards: Pure Chemistry ('58), Baekeland Medal ('59), Fritzsche Award ('60), Award for Creative Invention ('73); Freedman Found. Patent Award ('71) and Chem. Pioneer Award ('73) of Am.Inst.Chem.; Intrascience Res. Found. Award ('69); Hon. Member and Centenary Lecturer, Chem.Soc.(London); (continued below)

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Natural Products Chemistry and chemical applications of physical methods	Principal Investigator

RESEARCH SUPPORT *(See instructions)*

See attached.

HONORS (continued from above): Member of National Academy of Sciences, American Academy of Arts and Sciences, Royal Swedish Academy of Sciences, German Academy of Natural Scientists (leopoldina), Honorary D. Sc. Kenyon, Mexico, Rio de Janeiro, Worcester Polytechnic, Wayne State.

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Academic Experience

Professor of Chemistry, Stanford University, 1959-present
Assoc. Professor ('52-'54) and Professor ('54-'59), Wayne State University

Industrial Experience

Zoecon Corp., Palo Alto, Calif. Chairman of the Board and Chief Exec. Officer, '68-present
Syntex Corp.: Various positions in Mexico City ('49-'52, '57-'60) and Palo Alto, Calif. ('60-'72) ranging from Assoc. Director of Chemical Research to President of Syntex Research
Ciba Pharmaceutical Co., Summit, N.J., Research Chemist, '42-'43, '45-'49.

Miscellaneous

Chairman of AAAS Gordon Res. Conf. on Steroids and Nat. Prod. ('52-'54). Member Amer. Pugwash Committee ('68-'75); Chairman, Latin American Science Board of National Academy of Sciences ('66-'68); Member ('68-'72) and Chairman ('73-'75) of Board on Science and Technology for International Development of National Academy of Sciences; Member, President's Advisory Group on Contributions of Technology to Economic Strength.

Publications

Author or co-author of six books (four dealing with organic mass spectrometry) and over 800 scientific publications. A selection of those dealing with mass spectrometry is given in the Bibliography.

☆ U. S. GOVERNMENT PRINTING OFFICE : 1974 584-253/3034

RESEARCH SUPPORT: CARL DJERASSI

Agency: National Institutes of Health
Grant No.: GM-06840-18
Title of Grant: Marine Chemistry with Special Emphasis on Steroids
Period of Grant: 5/1/73-4/30/78
Current Budget: $101,490
Fraction of time committed: 15%

Agency: National Institutes of Health
Grant No.: AM-04257
Title of Grant: Mass Spectrometry in Organic and Biochemistry
Period of Grant: 10/1/75-9/30/79
Current Budget: $278,400
Fraction of time committed: 10%

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
JOSHUA LEDERBERG	Professor and Chairman Department of Genetics	5/23/25
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Montclaire, New Jersey, U.S.A.	U. S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Columbia College, New York	B.A.	1944	
College of Physicians & Surgeons, Columbia Univ., New York (1944-46)			
Yale University	Ph.D.	1947	Microbiology

HONORS

1957 - National Academy of Sciences
1958 - Nobel Prize in Medicine

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Molecular Genetics; Artificial Intelligence	Investigator

RESEARCH SUPPORT *(See instructions)*

Please see attached list.

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1959 - present Professor and Chairman, Department of Genetics
Stanford University School of Medicine

1957 - 1959 Chairman, Department of Medical Genetics
University of Wisconsin

1947 - 1957 Professor of Genetics
University of Wisconsin

Selected publications appear in Bibliography Section.

☆ U. S. GOVERNMENT PRINTING OFFICE : 1974 584-253/3034

Privileged Communication - Section II

Lederberg, Joshua

RESEARCH SUPPORT

GRANT NO.	TITLE OF PROJECT	CURRENT YEAR	PROJECT PERIOD	% OF EFFORT	GRANT AGENCY
Dr. Lederberg: personal research commitments					
5ROI CA16896-18	Genetics of Bacteria	$70,000 5/76-4/77	$195,000 5/74-4/77	15	NIH
NAS1-9692	Viking Mission Participation	$42,500 1/76-6/76	$62,572 1/75-3/77	5	NASA
Dr. Lederberg also functions as Principal Investigator ex officio on the following program-projects and training grants:					
NGR-05-020-632	Analytical Methodology for Biochemical Monitoring	$60,000 5/75-4/76	$180,000 5/73-4/76	2	NASA
NO1 CB 43902	Biomedical Markers that May Presage the Presence of Cancer	$95,000 6/75-6/76	$183,108 6/74-6/76	5	NIH
3TOI GM00295	Genetics Training Grant (graduate research training)	$121,000 7/75-6/76	$916,637 7/74-6/79	10	NIH
1T22 GM00198-02	Postdoctoral Training Medical Genetics	$48,133 7/75-6/76	$144,133 7/74-6/77	5	NIH
1PO7 RR00785-03	Stanford University Medical Experimental Computer: National Computer Resource for Research on AI in Medicine	$358,000 8/75-7/76	$3,092,226 10/73-7/78	10	NIH
NGR-05-020-004	Instrumentation for Planetary Exploration	$110,000 9/75-8/76	$110,000 9/75-8/76	5	NASA
GM20832-02	Genetics Research Project	$241,432 5/76-4/77	$1,292,113 5/74-4/79	10	NIH

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
EDWARD A. FEIGENBAUM	PROFESSOR OF COMPUTER SCIENCE	1-20-36
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Weehawken, New Jersey, U.S.A.	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Carnegie Institute of Technology Pittsburgh, Pennsylvania	B.S.	1956	Electrical Engineering
Carnegie Institute of Technology	Ph.D.	1959	Industrial Administration

HONORS

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Artificial Intelligence	Investigator

RESEARCH SUPPORT *(See instructions)*

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Stanford University, Stanford, California
- Chairman, Computer Science Department, 9/1976-
- Professor of Computer Science, 1969-
- Associate Professor of Computer Science, 1965-68
- Director, Stanford Computation Center, 1965-68

University of California, Berkeley
- Associate Professor, School of Business Administration, 1964
- Assistant Professor, School of Business Administration, 1960-63
- Research Appointment, Center for Human Learning, 1961-64
- Research Appointment, Center for Research in Management Science, 1960-64

Editor, Computer Science Series, McGraw-Hill Book Company, New York, 1965-

Member, Computer and Biomathematical Sciences Study Section, National Institutes of Health, Bethesda, Maryland, 1968-72

Ad-Hoc Mail Reviewer, National Science Foundation (various)

☆ U. S. GOVERNMENT PRINTING OFFICE : 1974 584-253/3034

Selected Papers, 1965-76

1. J. Lederberg and E. A. Feigenbaum, "Mechanization of Inductive Inference in Organic Chemistry", in B. Kleinmuntz (ed.), Formal Representations for Human Judgment, (Wiley, 1968). (Also Stanford Artificial Intelligence Project Memo No. 54, August 1967).

2. J. Lederberg, G. L. Sutherland, B. G. Buchanan, E. A. Feigenbaum, A. V. Robertson, A. M. Duffield, and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference I. The Number of Possible Organic Compounds: Acyclic Structures Containing C, H, O and N". Journal of the American Chemical Society, 91:11 (May 21, 1969).

3. B. G. Buchanan, G. L. Sutherland, E. A. Feigenbaum, "Toward an Understanding of Information Processes of Scientific Inference in the Context of Organic Chemistry", in Machine Intelligence 5, (B. Meltzer and D. Michie, eds.) Edinburgh University Press (1970). (Also Stanford Artificial Intelligence Project Memo No. 99, September 1969.)

4. E. A. Feigenbaum, B. G. Buchanan, and J. Lederberg, "On Generality and Problem Solving: A Case Study Using the DENDRAL Program". In Machine Intelligence 6 (B. Meltzer and D. Michie, eds.) Edinburgh University Press (1971). (Also Stanford Artificial Intelligence Project Memo No. 131.)

5. B. G. Buchanan, E. A. Feigenbaum, and J. Lederberg, "A Heuristic Programming Study of Theory Formation in Science." In Proceedings of the Second International Joint Conference on Artificial Intelligence, Imperial College, London (September, 1971). (Also Stanford Artificial Intelligence Project Memo No. 145.)

6. B. G. Buchanan, E. A. Feigenbaum, and N. S. Sridharan, "Heuristic Theory Formation: Data Interpretation and Rule Formation". In Machine Intelligence 7, Edinburgh University Press (1973).

7. D. H. Smith, B. G. Buchanan, W. C. White, E. A. Feigenbaum, C. Djerassi and J. Lederberg, "Applications of Artificial Intelligence for Chemical Inference X. INTSUM. A Data Interpretation Program as Applied to the Collected Mass Spectra of Estrogenic Steroids". Tetrahedron, 29, 3117 (1973).

8. E. A. Feigenbaum, "Computer Applications: Introductory Remarks," in Proceedings of Federation of American Societies for Experimental Biology, Vol. 33, No. 12 (Dec., 1974) 2331-2332.

Other papers in Information Processing Psychology (18)

Books and Monographs

1. Computers and Thought, co-editor with Julian Feldman, McGraw-Hill, 1963.

2. Information Processing Language V Manual, Englewood Cliffs, N.J., Prentice-Hall, 1961 (with A. Newell, F. Tonge, G. Mealy, et.al.).

3. An Information Processing Theory of Verbal Learning, Santa Monica, The RAND Corporation Paper P-1817, October 1959 (monograph).

RESEARCH SUPPORT AND PENDING APPLICATIONS: Edward A. Feigenbaum

Agency: Advanced Research Projects Agency
Contract Number: DAHC 15 73 C 0435
Title of Contract: Heuristic Programming Project
Period of Contract: July 1975-June 1977
Annual Budget Level: $203,000
Fraction of time committed: 40% Academic Yr.

Agency: National Science Foundation
Grant Number: MCS 76-11649
Title of Grant: MOLGEN: A Computer Science Application to Molecular Genetics
Period of Grant: 6/1/76-5/31/78
Annual Budget Level: $110,700 (2 yr. amount)
Fraction of time committed: 10% Academic Yr.; 100% Summer

PENDING:

Agency: National Library of Medicine
Title: Training Program in Biomedical Computing
Period: 6/77-5/82
Annual Budget Level: $334,193 (direct cost)
Fraction of time committed: 20%

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
BRUCE G. BUCHANAN	Adjunct Professor	7-7-40
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
St. Louis, Missouri, U.S.A.	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Ohio Wesleyan University	B.A.	1961	Mathematics
Michigan State University	M.A.	1966	Philosophy
Michigan State University	Ph.D.	1966	Philosophy

HONORS
Recipient of National Institutes of Health Career Development Award (1971-1976); Invited Speaker: 1975 NATO Advanced Study Institute on Machine Representation of Knowledge; 1974 Gordon Conference on Scientific Information Problems in Research.

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
	Associate Investigator

RESEARCH SUPPORT *(See instructions)*

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1976 - Adjunct Professor, Computer Science Department
Stanford University, Stanford, California

1972-1976 Research Computer Scientist, Computer Science Department
Stanford University, Stanford, California

1966-1971 Research Associate, Artificial Intelligence Project
Stanford University, Stanford, California

☆ U. S. GOVERNMENT PRINTING OFFICE : 1974 584-253/3034

Selected Publications:

1. B. G. Buchanan, "Applications of Artificial Intelligence to Scientific Reasoning." In Proceedings of Second USA-Japan Computer Conference, August, 1975.

2. E. H. Shortliffe, R. Davis, S. G. Axline, B. G. Buchanan, C. C. Green, and S. N. Cohen, "Computer-Based Consultations in Clinical Therapeutics: Explanation and Rule Acquisition Capabilities of the MYCIN System," Computers and Biomedical Research, 8, 303-320 (1975).

3. E. H. Shortliffe and B. G. Buchanan, "A Model of Inexact Reasoning in Medicine", Mathematical Biosciences, 23, 351-379 (1975).

4. D. Michie and B. G. Buchanan, "The Scientist's Apprentice" in Computers for Spectroscopy (ed. R.A.G. Carrington) London: Adam Hilger, 1974.

5. B. G. Buchanan and N. S. Sridharan, "Rule Formation on Non-Homogeneous Classes of Objects". Proceedings of the Third International Joint Conference on Artificial Intelligence (1973).

6. D. H. Smith, B. G. Buchanan, W. C. White, E. A. Feigenbaum, C. Djerassi, and J. Lederberg, "Applications of Artificial Intelligence for Chemical Inference X. Intsum. A Data Interpretation Program as Applied to the Collected Mass Spectra of Estrogenic Steroids". Tetrahedron, 29, 3117 (1973).

7. D. H. Smith, B. G. Buchanan, R. S. Engelmore, H. Aldercreutz and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference IX. Analysis of Mixtures Without Prior Separation as Illustrated for Estrogens". Journal of the American Chemical Society, 95, 6078, 1973.

8. B. G. Buchanan, Review of Hubert Dreyfus' "What Computers Can't Do: A Critique of Artificial Reason", Computing Reviews (January, 1973).

9. B. G. Buchanan, E. A. Feigenbaum and N. S. Sridharan, "Heuristic Theory Formation: Data Interpretation and Rule Formation". Machine Intelligence 7, Edinburgh University Press (1972).

10. C. W. Churchman and B. G. Buchanan, "On the Design of Inductive Systems: Some Philosophical Problems". British Journal for the Philosophy of Science, 20 (1969), 311-323.

11. B. G. Buchanan, G. L. Sutherland, E. A. Feigenbaum, "Toward an Understanding of Information Processes of Scientific Inference in the Context of Organic Chemistry", Machine Intelligence 5 (B. Meltzer and D. Michie, eds.), Edinburgh University Press (1970). (Also Stanford Artificial Intelligence Project Memo No. 99, September 1969.)

RESEARCH SUPPORT AND PENDING APPLICATIONS: Bruce G. Buchanan

Agency: Advanced Research Projects Agency
Contract Number: DAHC 15 73 C 0435
Title of Contract: Heuristic Programming Project
Period of Contract: July 1975-June 1977
Annual Budget Level: $203,000
Fraction of time committed: 25%

Agency: National Science Foundation
Grant Number: MCS 76-11649
Title of Grant: MOLGEN: A Computer Science Application to Molecular Genetics
Period of Grant: 6/1/76-5/31/78
Annual Budget Level: $110,700 (2 yr. amount)
Fraction of time committed: 25%

PENDING:

Agency: National Library of Medicine
Title: Training Program in Biomedical Computing
Period: 6/77-5/82
Annual Budget Level: $334,193 (direct cost)
Fraction of time committed: 20%

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Dennis H. Smith	Research Associate	11/12/42

PLACE OF BIRTH *(City, State, Country)*	PRESENT NATIONALITY *(If non-U.S. citizen, indicate kind of visa and expiration date)*	SEX
New York	USA	X Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Massachusetts Inst. of Technology Cambridge, Mass.	S.B.	1964	Chemistry
University of California, Berkeley Berkeley, California	Ph.D.	1967	Chemistry

HONORS

Alfred P. Sloan Foundation Scholarship
NASA Predoctoral Traineeship
Phi Lambda Upsilon, Sigma Xi

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Mass Spectrometry and A.I. in Chemistry	Research Associate

RESEARCH SUPPORT *(See instructions)*

N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1971-Present Research Associate, Stanford University, Stanford,Ca.
1970-1971 Visiting Scientist, University of Bristol, Bristol, England
1967-1970 Assistant Research Chemist, University of Calif.at Berkeley, Berkeley, Ca.
1965-1967 NASA Pre-Doctoral Traineeship, University of Calif.at Berkeley,Berkeley, Ca.

Publications: See attached list.

DENNIS H. SMITH Selected Publications

1. H.G. Langer, R.S. Gohlke, and D.H. Smith, "Mass Spectrometric Differential Thermal Analysis," Anal. Chem., 37, 433 (1965).

2. S.M. Kupchan, J.M. Cassady, J.E. Kelsey, H.K. Schnoes, D.H. Smith, and A.L. Burlingame, "Structural Elucidation and High Resolution Mass Spectrometry of Gaillardin, a New Cytotoxic Sesquiterpene Lactone," J. Amer. Chem. Soc., 88, 5292 (1966).

3. D.H. Smith, Ph.D. Thesis, "High Resolution Mass Spectrometry: Techniques and Applications to Molecular Structure Problems," Dept. of Chemistry, University of California, Berkeley, California (1967).

4. H.K. Schnoes, D.H. Smith, A.L. Burlingame, P.W. Jeffs, and W. Dopke, "Mass Spectra of Amaryllidaceae Alkaloids: The Lycorenine Series," Tetrahedron, 24, 2825 (1968).

5. A.L. Burlingame, D.H. Smith, and R.W. Olsen, "High Resolution Mass Spectrometry in Molecular Structure Studies. XIV. Real-time Data Acquisition, Processing and Display of High Resolution Mass Spectral Data," Anal. Chem., 40, 13 (1968).

6. A.L. Burlingame and D.H. Smith, "High Resolution Mass Spectrometry in Molecular Structure Studies. II. Automated Heteroatomic Plotting as an Aid to the Presentation and Interpretation of High Resolution Mass Spectral Data," Tetrahedron, 24, 5749 (1968).

7. W.J. Richter, B.R. Simoneit, D.H. Smith, and A.L. Burlingame, "Detection and Identification of Oxocarboxylic and Dicarboxylic Acids in Complex Mixtures by Reductive Silylation and Computer-Aided Analysis of High Resolution Mass Spectral Data," Anal. Chem., 41, 1392 (1969).

8. The Lunar Sample Preliminary Examination Team, "Preliminary Examination of Lunar Samples from Apollo 11," Science, 165, 1211 (1969).

9. S.M. Kupchan, W.K. Anderson, P. Bollinger, R.W. Doskotch, R.M. Smith, J.A. Saenz-Renauld, H.K. Schnoes, A.L. Burlingame, and D.H. Smith, "Tumor Inhibitors. XXXIX. Active Principles of Acnistus arborescens. Isolation and Structural and Spectral Studies of Withaferin A and Withacnistin," J. Org. Chem., 34, 3858 (1969).

10. A.L. Burlingame, D.H. Smith, T.O. Merren, and R.W. Olsen, "Real-time High Resolution Mass Spectrometry," in Computers in Analytical Chemistry (Vol. 4 in Progress in Analytical Chemistry series), C.H. Orr and J. Norris, Eds., Plenum Press, New York, 1970, pp. 17.

11. The Lunar Sample Preliminary Examination Team, "Preliminary Examination of Lunar Samples from Apollo 12," Science, 167, 1325 (1970).

12. D.H. Smith, "Mass Spectrometry," Chapter X in Guide to Modern Methods of Instrumental Analysis, T.M. Gouw, Ed., Wiley-Interscience, New York, 1972.

13. D.H. Smith, R.W. Olsen, F.C. Walls, and A.L. Burlingame, "Real-time Mass Spectrometry: LOGOS--A Generalized Mass Spectrometry Computer System for High and Low Resolution, GC/MS and Closed-Loop Applications," Anal. Chem., 43, 1796 (1971).

14. A.L. Burlingame, J.S. Hauser, B.R. Simoneit, D.H. Smith, K. Biemann, N. Mancuso, R. Murphy, D.A. Flory, and M.A. Reynolds, "Preliminary Organic Analysis of the Apollo 12 Cores," Proceedings of the Apollo 12 Lunar Science Conference, E. Levinson, Ed., M.I.T. Press, Cambridge, Mass., 1971, p. 1891.

15. D.H. Smith, "A Compound Classifier Based on Computer Analysis of Low Resolution Mass Spectral Data," Anal. Chem., 44, 536 (1972).

16. D.H. Smith and G. Eglinton, "Compound Classification by Computer Treatment of Low Resolution Mass Spectra-Application to Geochemical and Environmental Problems," Nature, 235, 325 (1972).

17. D.H. Smith, N.A.B. Gray, C.T. Pillinger, B.J. Kimble, and G. Eglinton, "Complex Mixture Analysis - Geochemical and Environmental Applications of a Compound Classifier Based on Computer Analysis of Low Resolution Mass Spectra," Adv. in Org. Geochem., 1971, p. 249.

18. P. Longevialle, D.H. Smith, H.M. Fales, R.J. Highet, and A.L. Burlingame, "High Resolution Mass Spectrometry in Molecualr Structure Studies. V. The Fragmentation of Amaryllis Alkaloids in the Crinine Series," Org. Mass. Spectrom., 7, 401 (1973).

19. B.R. Simoneit, D.H. Smith, G. Eglinton, and A.L. Burlingame, "Applications of Real-time Mass Spectrometric Techniques to Environmental Organic Geochemistry. II. San Francisco Bay Area Waters," Arch. Env. Contam. Tox., 1, 193 (1973).

20. G. Loew, M. Chadwick, and D.H. Smith, "Applications of Molecular Orbital Theory to the Interpretation of Mass Spectra. Prediction of Primary Fragmentation Sites in Organic Molecules," Org. Mass Spectrom., 7, 1241 (1973).

21. J.H. Block, D.H. Smith and C. Djerassi, "Mass Spectrometry in Structural and Stereochemical Problems, CCXXXVIII. The Effect of Heteroatoms upon the Mass Spectrometric Fragmentation of Cyclohexanones," J. Org. Chem., 39, 279 (1974).

22. D.H. Smith, C. Djerassi, K.H. Maurer, and U. Rapp, "Mass Spectrometry in Structural and Stereochemical Problems. CCXLII. Analysis of Mixtures Based on the Distribution of Fragment Ions Arising from Unimolecular Decomposition of Metastable Parent Ions," J. Amer. Chem. Soc., 96, 3482 (1974).

23. D.H. Smith, "The Scope of Structural Isomerism," J. Chem. Inf. Comp. Sci., 15, 203 (1975).

24. B.R. Simoneit, D.H. Smith, and G. Eglinton, "Application of Real-Time Mass Spectrometric Techniques to Environmental Organic Geochemistry. I. Computerized High Resolution Mass Spectrometry and Gas Chromatography-Low Resolution Mass Spectrometry," Arch. Environ. Cont. Tox., 3, 385 (1976).

25. T.R. Varkony, R.E. Carhart, and D.H. Smith, "Computer-Assisted Structure Elucidation. Modelling Chemical Reaction Sequences Used in Molecular Structure Problems," in "Computer-Assisted Organic Synthesis," W.T. Wipke, Ed., American Chemical Society, Washington, D.C., in press.

26. D.H. Smith and R.E. Carhart, "Structural Isomerism of Mono- and Sesquiterpenoid Skeletons," Tetrahedron, in press.

27. L.L. Dunham, C.A. Henrick, D.H. Smith, and C. Djerassi, "Mass Spectrometry in Structural and Stereochemical Problems. CCXLVI. Electron Impact Induced Fragmentation of Juvenile Hormone Analogs," Org. Mass Spectrom., in press.

See also Bibliography.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
RAYMOND EDGAR CARHART	RESEARCH ASSOCIATE	10/4/46
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Evanston, Illinois, U.S.A.	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Northwestern University	B.A.	1968	Chemistry
California Institute of Technology	Ph.D.	1973	Physical Organic Chemistry

HONORS

Phi Beta Kappa; Sigma Xi; Phi Lambda Upsilon; NSF pre-doctoral fellowship 1968-72; NIH post-doctoral fellowship 1972-74.

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Applications of Computer Science to Organic Chemistry	Research Associate

RESEARCH SUPPORT *(See instructions)*

N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1974- Research Associate, Department of Computer Science, Stanford University

1972-1974 NIH Post-doctoral Fellow, Department of Computer Science, Stanford University

1969(summer) Visiting Scientist, IBM Research Laboratory, San Jose, California

Recent Publications:

R. Carhart and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference XI: The Analysis of C13 NMR Data for Structure Elucidation of Acyclic Amines", Journal of the Chemical Society (Perkin II), 1753 (1973).

L. Masinter, N.S. Sridharan, R. Carhart and D.H. Smith, "Applications of Artificial Intelligence for Chemical Inference. XIII. Labeling of Objects Having Symmetry". Journal of the American Chemical Society, 96, 7714 (1974).

R. E. Carhart, D. H. Smith, H. Brown and N. S. Sridharan, "Applications of Artificial Intelligence for Chemical Inference. XVI. Computer Generation of Vertex Graphs and Ring Systems". Journal of Chemical Information and Computer Science, 15, 124 (1975).

R. E. Carhart, D. H. Smith, H. Brown and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference. XVII. An Approach to Computer-Assisted Elucidation of Molecular Structure". Journal of the American Chemical Society, 97, 5755 (1975).

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RAYMOND E. CARHART RECENT PUBLICATIONS

R. E. Carhart, S. M. Johnson, D. H. Smith, B. G. Buchanan, R. G. Dromey, J. Lederberg, "Networking and a Collaborative Research Community: A Case Study Using the DENDRAL Program," in "Computer Networking and Chemistry", P. Lykos, Ed., American Chemical Society, Washington, D.C., 1975, p. 192.

R. E. Carhart and D. H. Smith, "Applications of Artificial Intelligence for Chemical Inference. XX. 'Intelligent' Use of Constraints in Computer-Assisted Structure Elucidation," Computers in Chemistry, in press.

T. R. Varkony, R. E. Carhart, and D. H. Smith, "Computer-Assisted Structure Elucidation. Modelling Chemical Reaction Sequences Used in Molecular Structure Problems," in "Computer-Assisted Organic Synthesis," W. T. Wipke, Ed., American Chemical Society, Washington, D.C., in press.

D. H. Smith and R. E. Carhart, "Structural Isomerism of Mono- and Sesquiterpenoid Skeletons," Tetrahedron, in press.

R. E. Carhart, "A Model-Based Approach to the Teletype Printing of Chemical Structures," Journal of Chemical Information and Computer Science, in press.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Gretchen Maria SCHWENZER	Research Associate	2/6/49

PLACE OF BIRTH *(City, State, Country)*	PRESENT NATIONALITY *(If non-U.S. citizen, indicate kind of visa and expiration date)*	SEX
Buffalo, New York, U.S.A.	U.S.	☐ Male ☒ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
State University of New York at Buffalo	B.A.	1971	Mathematics & Chemistry
University of California, Berkeley	Ph.D.	1975	Chemistry
Institute in Quantum Chemistry, Solid State Physics & Quantum Biology, Uppsala, Sweden		Summer 1973	

HONORS

Phi Beta Kappa, Pi Mu Epsilon, Alpha Lambda Delta
Graduated Magna Cum Laude with Highest Distinction; Allied Chemical Scholar, 1971; Award of American Institute of Chemists for Scholastic Achievement.

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Application of Computers in Chemistry	Direct C13 NMR with attention to the structural nature of the problem

RESEARCH SUPPORT *(See instructions)*

N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Stanford University 1976 -
Computer Science Department, Stanford, Calif.

IBM, San Jose Research Division, San Jose, Calif. 1975

University of California, Berkeley, Calif. 1971-1975

Thesis: The Excited Electronic States of HCN and HNC; a New Method to Obtain Wave Functions of SCF Quality Configuration Interaction Wave Functions to Obtain Optimized Minimum Basis Set Potential Surfaces

State University of New York at Buffalo, Buffalo, N.Y.

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"Photochemical Substitution Reactions of Substituted Group VI Metal Carbonyls," G. Schwenzer, M.Y. Darensbourg, and D.J. Darensbourg, Inorganic Chemistry, 11, 1967 (1972).

"Photochemical Substitution Reactions of Substituted Group VI Metal Carbonyls," G. Schwenzer, D.J. Darensbourg, M.Y. Darensbourg, ACS Meeting, New York, Aug. (1972).

"Use of nonrelativistic wavefunctions for the prediction of properties of molecules containing atoms of high Z. PbO as a test case," Gretchen M. Schwenzer, Dean H. Liskow, and Henry F. Schaefer, The Journal of Chemical Physics, Vol. 58, No. 8, 15 April 1973.

"Geometries of the excited electronic states of HCN," Gretchen M. Schwenzer, Stephen V. O'Neil, and Henry F. Schaefer, The Journal of Chemical Physics, Vol. 60, No. 7, 1 April 1974.

"The Hypervalent Molecules Sulfurane (SH_4) and Persulfurane (SH_6)," Gretchen M. Schwenzer and Henry F. Schaefer, The Journal of the American Chemical Society, 97, 1393 (1975).

"Excited Electronic States of HNC, Hydrogen Isocyanide," Gretchen M. Schwenzer, Henry F. Schaefer, and Charles F. Bender, The Journal of Chemical Physics, 63, 569 (1975).

"Confirmation of the Discrepancy Between Theory and Experiment for the $B\ ^1A''$ state of HCN," Gretchen M. Schwenzer, Henry F. Schaefer and Charles F. Bender, Chemical Physics Letters, Vol. 36, No. 2, 179 (1975).

"Documentation of ALCHEMY", Gretchen M. Schwenzer, IBM Report.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
HAROLD D. BROWN	Research Associate	7-12-34
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
South Bend, Indiana, U.S.A.	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
University of Notre Dame	M.Sc.	1963	Mathematics
Ohio State University	Ph.D.	1966	Mathematics

HONORS

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
	Research Associate

RESEARCH SUPPORT *(See instructions)*

Pending, "Computer-Assisted Molecular Structure Elucidation", 12-month grant.
Proposed Amount: $42,733
Period: 11/1/75-10/31/77
Source: National Science Foundation

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1971-72 1973-	Associate Professor, Computer Science Department, Stanford University
1973-	Research Associate, Medical School, Stanford University
1963-75	Instructor/Assistant Professor, Assistant Chairman/Associate Professor, Mathematics, The Ohio State University
Winter 1971, 73 and 75	Visiting Professor, Mathematics, Rhine. Westf. Tech. Hoch., Aschen
1964-70	Director/Associate Director, National Science Foundation SSTP
1967-68	Visiting Member, Courant Institute of Mathematical Sciences, New York University
1960-63	Assistant to the Chairman, Mathematics, University of Notre Dame

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Publications:

Near Algebras, Ill. J. Math. 12(1968), p. 215.

Distributor Theory in Near Algebras, Comm. Pure Appl. Mat. XXI(1968), p. 535.

An Algorithm for the Determination of Space Groups, Math. Comp. 23(1969), p. 499.

Some Empirical Observations on Primitive Roots (with H. Zassenhaus), J. Number Theory 3(1971), p. 306.

A Generalization of Farey Sequences (with K. Mahler), J. Number Theory 3(1971), p. 364.

Basic Computations for Orders, Stanford CS Report STAN-CS-72-208.

An Application of Zassenhaus' Unit Theorem, Acta Arith. XX(1972), p. 154.

Integral Groups I: The Reducible Case (with J. Neubuser and H. Zassenhaus), Numer. Math. 19(1972), p. 386.

Integral Groups II: The Irreducible Case (with J. Neubuser and H. Zassenhaus), Numer. Math. 20(1972), p. 22.

Integral Groups III: Normalizers (with J. Neubuser and H. Zassenhaus), Math. Comp. 27(1973), p. 167.

Constructive Graph Labeling via Double Cosets (with L. Hjelmeland and L. Masinter), Discrete Math. 7(1973), p. 1; and Stanford CS Report STAN-CS-72-318.

An Algorithm for the Construction of the Graphs of Organic Molecules (with L. Masinter), Discrete Math. 8(1974), p. 227; and Stanford CS Report STAN-CS-73-261.

The Crystallographic Groups of 4-dimensional Space (with J. Neubuser, H. Wondratschek and H. Zassenhaus), Wiley Interscience (in preparation).

Molecular Structure Elucidation III: Fragment Embedding, Soc. Industrial and Applied Math. J. on Computing (submitted), and Stanford CS Report STAN-CS-74-469.

Applications of Artificial Intelligence for Chemical Inference XVII. Computer Generation of Vertex Graphs and Ring Systems (with R. Carhart, N. Sridharan and D. Smith), J. Chem. Inf. Comp. Sci. (in press).

Applications of Artificial Intelligence for Chemical Inference XVIII. An Approach to Computer-Assisted Elucidation of Molecular Structure (with R. Carhart and D. Smith), JACS (in press).

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